Electronic Supplementary Material (ESI) for Dalton Transactions.

Geometric and Electronic Structures of Five-Coordinate Manganese(II) "Picket Fence" Porphyrin Complexes

Supporting Information

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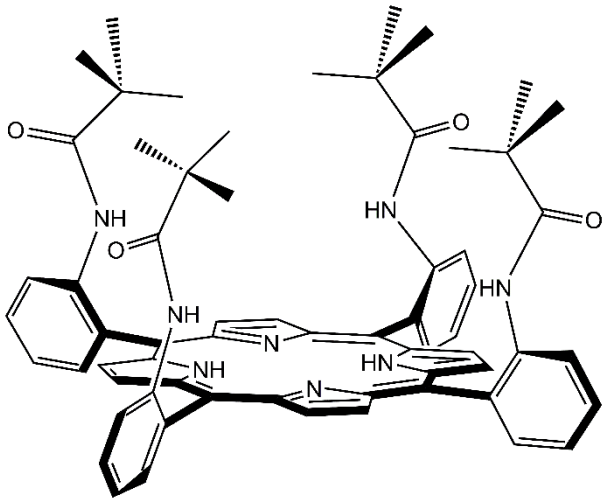

Figure S1. *α,α,α,α*-tetrakis(*o*-pivalamidophenyl)porphyrin

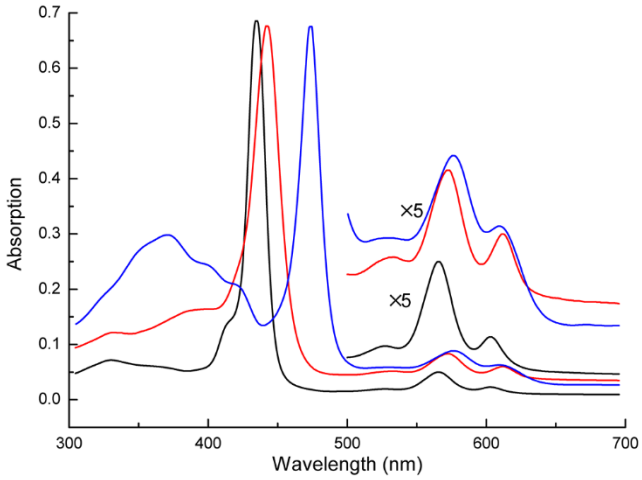

Figure S2. UV-vis spectrum of an anhydrous THF solution of [Mn(TpivPP)] (black line), [Mn(TpivPP)(1-MeIm)] (red line) and $[Mn(TpivPP)]_2O$ (blue line). The spectra from 500 to 700 nm are enlarged by 5 times.

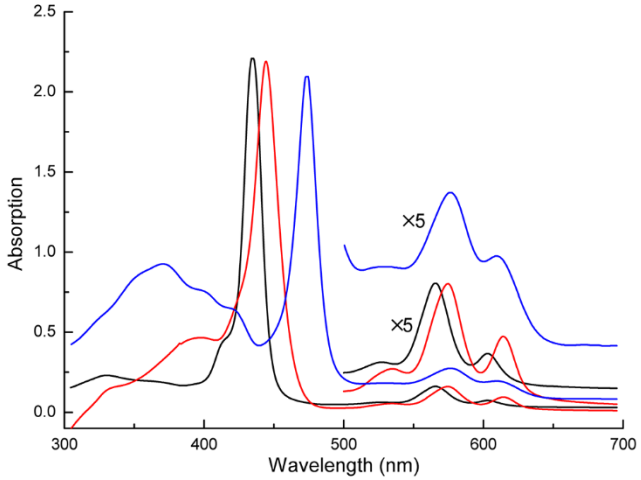

Figure S3. UV-vis spectrum of an anhydrous THF solution of [Mn(TpivPP)] (black line), [Mn(TpivPP)(1-EtIm)] (red line) and $[Mn(TpivPP)]_2O$ (blue line). The spectra from 500 to 700 nm are enlarged by 5 times.

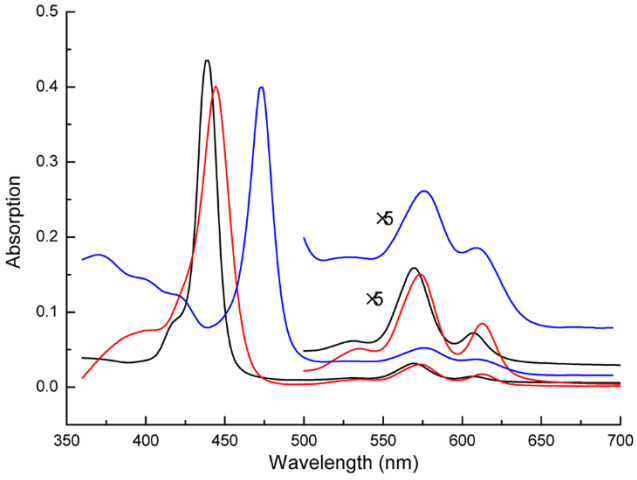

Figure S4. UV-vis spectrum of an anhydrous THF solution of [Mn(TpivPP)] (black line), [Mn(TpivPP)(2-MeHIm)] (red line) and $[Mn(TpivPP)]_2O$ (blue line). The spectra from 500 to 700 nm are enlarged by 5 times.

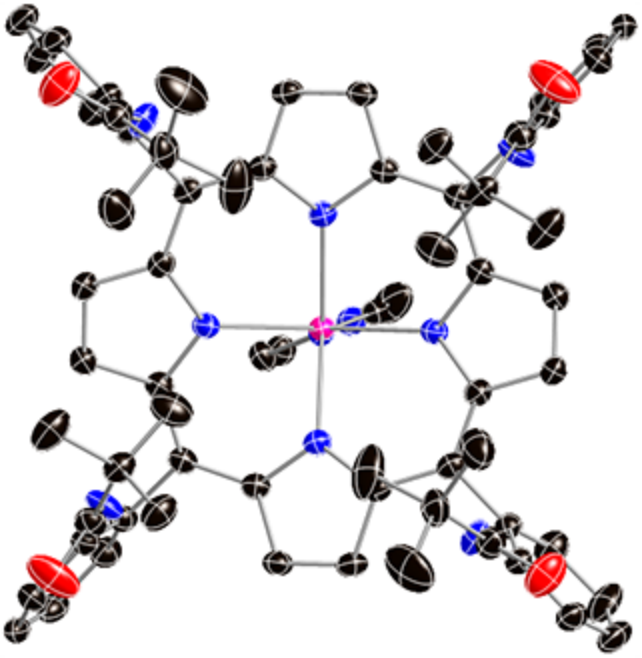

Figure S5. A top-down ORTEP diagram of [Mn(TpivPP)(1-MeIm)], Thermal ellipsoids are contoured at the 40% probability level. Hydrogen atoms omitted for clarity.

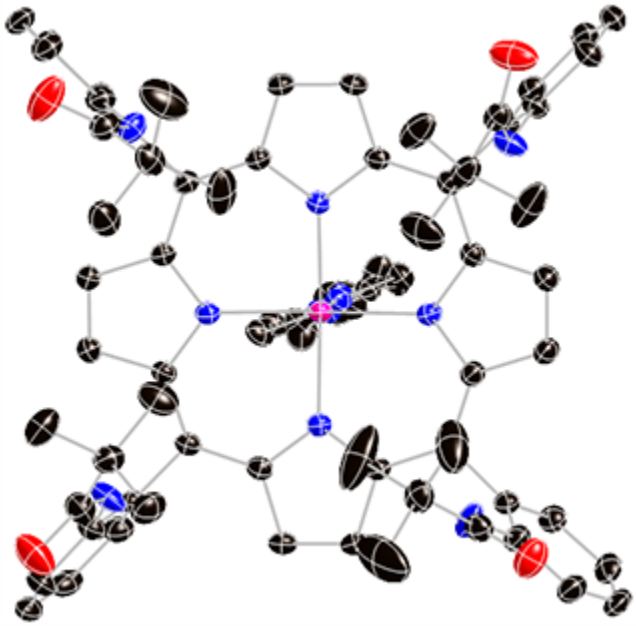

Figure S6. A top-down ORTEP diagram of [Mn(TpivPP)(1-EtIm)], Thermal ellipsoids are contoured at the 40% probability level. Hydrogen atoms omitted for clarity.

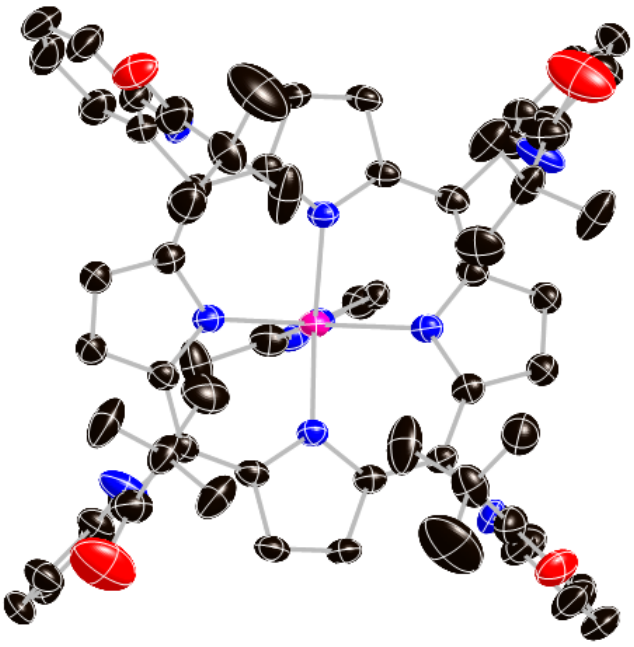

Figure S7. A top-down ORTEP diagram of [Mn(TpivPP)(2-MeHIm)], Thermal ellipsoids are contoured at the 40% probability level. Hydrogen atoms omitted for clarity.

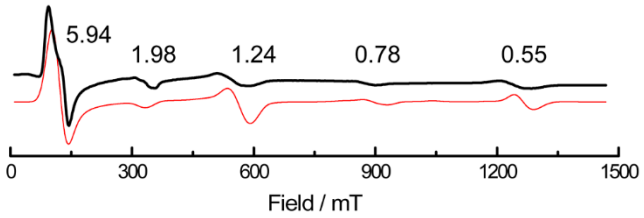

Figure S8. X-band EPR spectra (black line) and simulation (red line) of [Mn(TpivPP)(1-MeIm)] (a ground microcrystalline sample) at 90 K. EPR simulation conditions. (as follow)

Simulation conditions of X-band EPR spectra

[Mn(TpivPP)(1-MeIm)] (powder) Simulation conditions: S = 2.5, ^{55}Mn hyperfine coupling, g = 1.98, $A_{\perp}$ = 210 MHz, $A_{\parallel}$ = 270 MHz, D = 20250 MHz, E = 101.25 MHz.

[Mn(TpivPP)(2-MeHIm)] (powder) Simulation conditions: S = 2.5, ^{55}Mn hyperfine coupling, g = 1.98, $A_{\perp}$ = 220 MHz, $A_{\parallel}$ = 260 MHz, D = 20800 MHz, E = 104 MHz.

[Mn(TpivPP)(2-MeHIm)] (solution) Simulation conditions: S = 2.5, ^{55}Mn hyperfine coupling, g = 1.98, $A_{\perp}$ = 220 MHz, $A_{\parallel}$ = 260 MHz, D = 20200 MHz, E = 101 MHz.